What Is Claimed Is:

1. A method of selecting one or more compounds from a virtual combinatorial library associated with R reagent combinations, comprising the following steps:

    a.   selecting a first set of N reagent combinations from the R reagent combinations associated with the virtual combinatorial library, wherein $N < R$;

    b.   enumerating said first set of N reagent combinations to produce a first set of F enumerated compounds;

    c.   selecting M compounds from said first set of F enumerated compounds, wherein $M < F$;

    d.   deconvoluting said M compounds into reagents;

    e.   generating a focused library based on said reagents; and

    f.   enumerating a plurality of reagent combinations associated with said focused library to produce a second set of S enumerated compounds.

2. The method of claim 1, further comprising the step of:

    g.   selecting K compounds from said second set of S enumerated compounds, wherein $K < S$.

1 3. The method of claim 2, wherein step (g.) comprises selecting said K

2 compounds such that said K compounds can be produced using a predetermined

3 number T of reagents.

1 4. The method of claim 1, wherein step (a.) comprises selecting said first set of

2 N reagent combinations substantially at random from the virtual combinatorial

3 library.

1 5. The method of claim 1, wherein step (a.) comprises selecting said first set of

2 N reagent combinations such that a substantially uniform coverage of a reagent

3 space associated with the virtual combinatorial library is achieved.

1 6. The method of claim 1, wherein step (a.) comprises selecting said first set of

2 reagent combinations such that each reagent in the virtual combinatorial library is

3 selected a substantially equal number of times.

1 7. The method of claim 1, wherein step (c.) comprises selecting said M

2 compounds from said first set of F enumerated compounds based on a fitness

3 function.

1 8. The method of claim 7, further comprising the step of:

2   g.   selecting K compounds from said second set of S enumerated

3   compounds based on said fitness function, wherein $K < S$.

9. The method of claim 7, further comprising the step of:

    g.   selecting K compounds from said second set of S enumerated compounds based on said fitness function and such that said K compounds can be produced using a predetermined number T of reagents, wherein K < S.

10. The method of claim 8, wherein step (c) comprises

    i.   initially selecting M compounds from said first set of enumerated compounds to produce a first sub-set of enumerated compounds;

    ii.   evaluating said first sub-set of enumerated compounds based on said fitness function; and

    iii.   refining said first sub-set of enumerated compounds based on said fitness function.

11. The method of claim 10, wherein step (g.) comprises

    i.   initially selecting K compounds from said second set of enumerated compounds to produce a second sub-set of enumerated compounds;

    ii.   evaluating said second sub-set of enumerated compounds based on said fitness function; and

iii.   refining said second sub-set of enumerated compounds based on the fitness function.

12. The method of claim 11, wherein the fitness function is related to diversity of a collection of compounds, and wherein step (c.ii.) comprises evaluating the diversity of said first sub-set of enumerated compounds, and wherein step (c.iii.) comprises refining said first sub-set to increase the diversity of said first sub-set.

13. The method of claim 12, wherein step (g.ii.) comprises evaluating the diversity of said second sub-set of enumerated compounds, and wherein step (g.iii.) comprises refining said second sub-set to increase the diversity of said second sub-set.

14. The method of claim 8, wherein step (c.) comprises:

i.   characterizing each compound of said first set of enumerated compounds;

ii.   evaluating each characterized compound of said first set of enumerated compounds based on said fitness function;

iii.   ranking each characterized compound of said first set of enumerated compounds; and

iv.   selecting M compounds of said first set of enumerated compounds based on said ranking.

15. The method of claim 14, wherein step (g.) comprises:

    i.   characterizing each compound of said second set of enumerated compounds;

    ii.   evaluating each characterized compound of said second set of enumerated compounds based on said fitness function;

    iii.   ranking each characterized compound of said second set of enumerated compounds; and

    iv.   selecting K compounds of said second set of compounds based on said ranking.

16. The method of claim 15, wherein step (c.i.) comprises characterizing each compound of said first set of enumerated compounds using a set of molecular descriptors.

17. The method of claim 16, wherein step (g.i.) comprises characterizing each compound of said second set of enumerated compounds using said set of molecular descriptors.

18. The method of claim 15, wherein the fitness function is related to similarity to one or more query structures, and wherein step (c.ii.) comprises evaluating similarity between each compound of said first set of enumerated compounds and the one or more query structures.

19. The method of claim 18, wherein at least one of the following similarity measures is used in step (c.ii.) for evaluating similarity between each compound and the one or more query structures:

(1)   similarity in number of atoms, bonds and rings of the same types;

(2)   similarity in shape and surface characteristics;

(3)   similarity in electron density distribution;

(4)   similarity based on common substructure;

(5)   similarity based on the presence and orientation of pharmacophoric groups;

(6)   similarity in binding affinity; and

(7)   similarity in degree of conformational overlap with a know receptor binder.

20. The method of claim 18, wherein step (g.ii.) comprises evaluating similarity between each compound of said second set of enumerated compounds and the one or more query structures, and wherein the same similarity measure is used for evaluating similarity in step (c.ii.) and step (g.ii.).

21. The method of claim 14, wherein the fitness function is related to at least one desired characteristic, and wherein step (c.ii.) comprises evaluating each compound of said first set of enumerated compounds to determine an extent that each compound possesses the at least one desired characteristic.

22. The method of claim 21, wherein the at least one desired characteristic comprises at least one of the following:

     (1)   a desired physical property;

     (2)   a desired chemical property;

     (3)   a desired functional property; and

     (4)   a desired bioactive property.

23. A system for selecting, based on a fitness function, one or more compounds from a virtual combinatorial library associated with R reagent combinations, comprising:

means for selecting a first set of N reagent combinations from the R reagent combinations associated with the virtual combinatorial library, wherein R < N;

means for enumerating said first set of N reagent combinations to produce a first set of F enumerated compounds;

means for selecting M compounds of said first set of F enumerated compounds based on the fitness function, wherein M < F;

means for deconvoluting said M compounds into reagents;

means for generating a focused library based on said reagents;

means for enumerating a plurality of reagent combinations associated with said focused library to produce a second set of S enumerated compounds;

15   means for selecting K compounds of said second set of enumerated compounds

16   based on the fitness function, wherein $K < S$.

1   24. A computer program product comprising a computer useable medium having

2   computer program logic recorded thereon for enabling a processor to assist in

3   selecting, based on a fitness function, one or more compounds, from a virtual

4   combinatorial library associated with R regent combinations, the computer

5   program logic comprising:

6   means for enabling a processor to select a first set of N reagent combinations from

7   the R reagent combinations associated with the virtual combinatorial

8   library, wherein $N < R$;

9   means for enabling a processor to enumerate said first set of N reagent

10   combinations to produce a first set of F enumerated compounds;

11   means for enabling a processor to select M compounds of said first set of

12   enumerated compounds based on the fitness function, wherein $M < F$;

13   means for enabling a processor to deconvolute said M compounds into reagents;

14   means for generating a focused library based on said reagents;

15   means for enabling a processor to enumerate a plurality of reagent combinations

16   associated with said focused library to produce a second set of S

17   enumerated compounds; and

18   means for enabling a processor to select K compounds of said second set of

19   enumerated compounds based on the fitness function, wherein $K < S$.

25. A method of selecting one or more compounds from an enumerated virtual combinatorial library associated with R enumerated compounds, comprising the following steps:

    a.   selecting a first set of N enumerated compounds for the R enumerated compounds associated with the enumerated virtual combinatorial library, wherein $N < R$;

    b.   selecting M compounds from said first set of N enumerated compounds, wherein $M < N$;

    c.   deconvoluting said M compounds into reagents; and

    d.   using said reagents to extract an enumerated focused library from said enumerated virtual combinatorial library, said enumerated focused library including S enumerated compounds.

26. The method of claim 25, further comprising the step of:

    e.   selecting K compounds from said S enumerated compounds, wherein $K < S$.

27. The method of claim 26, wherein step (e.) comprises selecting said K compounds such that said K compounds can be produced using a predetermined number T of reagents.

1   28. The method of claim 25, wherein step (a.) comprises selecting said first set

2   of N enumerated compounds substantially at random from the enumerated virtual

3   combinatorial library.

1   29. The method of claim 25, wherein step (a.) comprises selecting said first set

2   of N enumerated compounds such that a substantially uniform coverage of a

3   reagent space associated with the enumerated virtual combinatorial library is

4   achieved.

1   30. The method of claim 25, wherein step (a.) comprises selecting said first set

2   of enumerated compounds such that each reagent in the enumerated virtual

3   combinatorial library is selected a substantially equal number of times.

1   31. The method of claim 25, wherein step (b.) comprises selecting said M

2   compounds from said first set of N enumerated compounds based on a fitness

3   function.

1   32. The method of claim 31, further comprising the step of:

2   e.   selecting K compounds from said S enumerated compounds based

3   on said fitness function, wherein K < S.

1   33. The method of claim 31, further comprising the step of:

2   e.   selecting K compounds from said S enumerated compounds based

3   on said fitness function and such that said K compounds can be

4   produced using a predetermined number T of reagents, wherein K

5   < S.

1   34. The method of claim 32, wherein step (b.) comprises

2   i.   initially selecting M compounds from said first set of

3   enumerated compounds to produce a first sub-set of

4   enumerated compounds;

5   ii.   evaluating said first sub-set of enumerated compounds

6   based on said fitness function; and

7   iii.   refining said first sub-set of enumerated compounds based

8   on said fitness function.

1   35. The method of claim 34, wherein step (e.) comprises

2   i.   initially selecting K compounds from said S enumerated

3   compounds to produce a second sub-set of enumerated

4   compounds;

5   ii.   evaluating said second sub-set of enumerated compounds

6   based on said fitness function; and

7   iii.   refining said second sub-set of enumerated compounds

8   based on said fitness function.

36. The method of claim 35, wherein the fitness function is related to diversity of a collection of compounds, and wherein step (b.ii.) comprises evaluating the diversity of said first sub-set of enumerated compounds, and wherein step (b.iii.) comprises refining said first sub-set to increase the diversity of said first sub-set.

37. The method of claim 36, wherein step (e.ii.) comprises evaluating the diversity of said S enumerated compounds, and wherein step (e.iii.) comprises refining said S enumerated compounds to increase the diversity of said S enumerated compounds.

38. The method of claim 32, wherein step (b.) comprises:

    i.   characterizing each compound of said first set of enumerated compounds;

    ii.   evaluating each characterized compound of said first set of enumerated compounds based on said fitness function;

    iii.   ranking each characterized compound of said first set of enumerated compounds; and

    iv.   selecting M compounds of said first set of enumerated compounds based on said ranking.

39. The method of claim 38, wherein step (e.) comprises:

    i.   characterizing each compound of said S enumerated compounds;

ii.   evaluating each characterized compound of said S

enumerated compounds based on said fitness function;

iii.   ranking each characterized compound of said S

enumerated compounds; and

iv.   selecting K compounds of said S enumerated compounds

based on said ranking.

40. The method of claim 39, wherein step (b.i.) comprises characterizing each compound of said first set of enumerated compounds using a set of molecular descriptors.

41. The method of claim 40, wherein step (e.i.) comprises characterizing each compound of said S enumerated compounds using said set of molecular descriptors.

42. The method of claim 38, wherein the fitness function is related to similarity to one or more query structures, and wherein step (b.ii.) comprises evaluating similarity between each compound of said first set of enumerated compounds and the one or more query structures.

43. The method of claim 42, wherein at least one of the following similarity measures is used in step (b.ii.) for evaluating similarity between each compound and the one or more query structures:

4   (1)   similarity in number of atoms, bonds and rings of

5   the same types;

6   (2)   similarity in shape and surface characteristics;

7   (3)   similarity in electron density distribution;

8   (4)   similarity based on common substructure;

9   (5)   similarity based on the presence and orientation of

10   pharmacophoric groups;

11   (6)   similarity in binding affinity; and

12   (7)   similarity in degree of conformational overlap with

13   a know receptor binder.

1   44. The method of claim 42, wherein step (e.ii.) comprises evaluating similarity

2   between each compound of said S enumerated compounds and the one or more

3   query structures, and wherein the same similarity measure is used for evaluating

4   similarity in step (b.ii.) and step (e.ii.).

1   45. The method of claim 38, wherein the fitness function is related to at least one

2   desired characteristic, and wherein step (b.ii.) comprises evaluating each

3   compound of said first set of enumerated compounds to determine an extent that

4   each compound possesses the at least one desired characteristic.

1   46. The method of claim 45, wherein the at least one desired characteristic

2   comprises at least one of the following:

3   (1)   a desired physical property;

4   (2)   a desired chemical property;

5   (3)   a desired functional property; and

6   (4)   a desired bioactive property.

1   47. A system for selecting, based on a fitness function, one or more compounds

2   from an enumerated virtual combinatorial library associated with R enumerated

3   compounds, comprising:

4   means for selecting a first set of N enumerated from the R enumerated compounds

5   associated with the enumerated virtual combinatorial library, wherein R <

6   N;

7   means for selecting M compounds of said first set of N enumerated compounds

8   based on the fitness function, wherein M < N;

9   means for deconvoluting said M compounds into reagents;

10   means for extracting an enumerated focused library, based on said reagents, from

11   the enumerated virtual combinatorial library, wherein said enumerated

12   focused library includes S enumerated compounds; and

13   means for selecting K compounds of said S enumerated compounds based on the

14   fitness function, wherein K < S.

1   48. A computer program product comprising a computer useable medium having

2   computer program logic recorded thereon for enabling a processor to assist in

3   selecting, based on a fitness function, one or more compounds, from an

4   enumerated virtual combinatorial library associated with R enumerated

5   compounds, the computer program logic comprising:

6   means for enabling a processor to select a first set of N enumerated compounds

7   from the R enumerated compounds associated with the enumerated virtual

8   combinatorial library, wherein N < R;

9   means for enabling a processor to select M compounds of said first set of

10 enumerated compounds based on the fitness function, wherein M < N;

11 means for enabling a processor to deconvolute said M compounds into reagents;

12 means for extracting an enumerated focused library, based on said reagents, from

13 the enumerated virtual combinatorial library, wherein said enumerated

14 focused library includes S enumerated compounds; and

15 means for enabling a processor to select K compounds of said S enumerated

16 compounds based on the fitness function, wherein K < S.